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Hybrid Modeling for Extrapolation and Transfer Learning in the Chemical Processing Industries

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Hybrid modeling is a class of methods that combines physics-based and data-driven models to achieve improved prediction performance, robustness, and explainability. It has attracted a significant amount of research and interest due to the increasing data availability and more powerful analytics and statistical methodologies (von Stosch et al., 2014; Sansana et al., 2021). In the context of the Chemical Processing Industries (CPI), hybrid modeling has the potential to improve the extrapolation capabilities of existing models. This is a critical activity for CPI as new process conditions, products, and product grades are manufactured to handle shifting trends in market demand, raw materials, and utility costs.
In this work, we study the application of hybrid modeling for supporting extrapolation and transfer learning, both critical tasks for CPI. We study different configurations of hybrid modeling (e.g., parallel, series) and compare them to benchmarks that include a physics-based model only and data-driven models only. The physics-based model considers simplified reaction kinetics. The set of data-driven methods includes partial least squares (PLS), least absolute shrinkage and selection operator (LASSO), random forest and boosting, support vector regression (SVR), and neural networks (NN). A simulated case study of biodiesel production (Fernandes et al., 2019) is considered, and hybrid modeling consistently shows improved results compared to using physics-based or data-driven models only. In particular, serial hybrid approaches are preferred for the extrapolation task. Regarding the transfer learning task, hybrid modeling also shows advantages, requiring fewer samples than other benchmarks.

Keywords

Hybrid Models, Transfer Learning, extrapolation

Classification

Both methodology and application

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